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Quantum chemical calculation of exchange interactions in supramolecularly arranged N,N′-dioxy-2-6-diazaadamantane organic biradical

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Abstract

Â© 2016 Wiley Periodicals, Inc.Quantum mechanical exchange effects in purely organic N,N′-dioxy-2,6-diazaadamantane biradical derivatives with promesogenic substituents have been studied. To determine intermolecular exchange energies, packing conditions of the radical core units in layered liquid crystalline phases are simulated using the Gaussian 09 program. The broken symmetry approach gives J ≈ 7 cm-1 for intramolecular ferromagnetic exchange interactions between nitroxyl radical centers in one molecule. Both ferromagnetic and antiferromagnetic intermolecular interactions are possible in this kind of systems according to the obtained calculation results. Depending on the mutual positioning and orientation of molecules, the intermolecular antiferromagnetic exchange constant can reach a value of -50 cm-1, and the intermolecular ferromagnetic constant a value of 10 cm-1. The simultaneous presence of intramolecular and intermolecular exchange between spin-carrying centers in this kind of supramolecularly ordered multispin systems is favorable for the formation of magnetically interacting chains and two-dimensional networks.

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Keywords

exchange interactions, N,N′-dioxy-2,6-diazaadamantane biradical, organic magnets, quantum chemical calculations, soft materials